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Characterization of point defects in CdTe by positron annihilation spectroscopy

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Positron lifetime measurements on CdTe 0.15% Zn-doped by weight are presented, trapping to monovacancy defects is observed. At low temperatures, localization at shallow binding energy positron traps dominates. To aid defect identification density functional theory, calculated positron lifetimes and momentum distributions are obtained using relaxed geometry configurations of the monovacancy defects and the Te antisite. These calculations provide evidence that combined positron lifetime and coincidence Doppler spectroscopy measurements have the capability to identify neutral or negative charge states of the monovacancies, the Te antisite, A-centers, and divacancy defects in CdTe. [http://dx.doi.org/10.1063/1.4953781]

Cadmium telluride has a bandgap of 1.5 eV, which provides an excellent match to the solar spectrum, and with the addition of Zn ($Cd_{1-x}Zn_xTe$), this value can be controllably increased. The relatively high average atomic number, and the ability to achieve high resistivity values, makes these materials ideal for gamma and x-ray detector devices. Further, CdTe can be doped both *n*- and *p*-type. However, material performance can be compromised by the presence of native and impurity ion point defects, influencing resistivity and hence detector efficiency, acting as carrier traps and recombination centers degrading photovoltaic device performance. Despite many decades of experimental studies, using a range of different techniques, routine detection and unambiguous identification of point defects in CdTe and related materials remains a challenge. However, increasingly accurate density functional theory (DFT) calculations are providing valuable insight on the nature and behavior of point defects in CdTe[1–4] and $Cd_{1-x}Zn_xTe$,[5,6] and these are, in turn, aiding the interpretation of experiments. The experimental methods that are capable of detecting point defects with a sensitivity better than $10^{16}\,cm^{-3}$, and which provide information on local structure, include the positron annihilation spectroscopy techniques.[7] These methods can unambiguously determine the presence of open volume point defects with neutral or negative local charge. The temperature dependence of positron trapping can determine the charge state of vacancy-related defects[8] and can also provide evidence on the presence of acceptor point defects without open volume such as substitutional impurities.[9]

The lifetime of the localized positron state is sensitive to the size of the open volume, and the chemical nature of the near neighbor atoms dominates the electron momentum distribution sampled by the positron in the high momentum region. These can be measured using positron annihilation lifetime spectroscopy (PALS) and coincidence Doppler broadening spectroscopy (CDBS), respectively, and the results from both can be compared to DFT calculations.[7]

Here, we present PALS results on $Cd_{1-x}Zn_xTe$ crystals with low x, and compare these with atomic superposition DFT calculations of positron lifetimes utilizing geometries obtained from recent DFT studies of point defects in CdTe.[1–4] The possibility of positron trapping to the vacancy-interstitial geometries obtained for the Te antisite and the effects of charge state and local structural relaxation of Cd vacancy related defects and the Te vacancy are investigated. The similarities in lifetime values between, for example, V_{Cd}^{-2} and Te_{Cd}^{0} motivate an extension of these calculations to CDBS ratio spectra.

Positron lifetime measurements were performed on $Cd_{1-x}Zn_xTe$ crystals,[10] grown using 0.15% Zn by weight, supplied by Kromek Group plc.[11] The crystals had approximately 1 ppm excess of Te and were low resistivity ($<1\times10^5\,\Omega$cm).[12] Measurements were performed with positron sources supported on 8 μm Kapton using conventional fast-fast coincidence spectrometers,[13] and the instrument resolution functions (IRF) were obtained from measurements on directly deposited aluminum before and after the sample measurements. Spectra contained greater than 5×10^6 counts. The room temperature measurements were performed using a spectrometer with a 203 ps full width half maximum (FWHM) IRF, variable temperature measurements using a system with a 265 ps FWHM IRF. Corrections for source annihilation events were performed assuming the known lifetime for Kapton foil,[14] and using the procedures outlined elsewhere.[13] Analysis was performed using the standard trapping model (STM).[7,15] The room temperature experimental PALS spectra from the CdTe:Zn crystals best fitted to two lifetime components, a defect component with a lifetime of 331(4) ps (intensity 86(1)%) and a reduced bulk component, giving a STM bulk lifetime of 290(4) ps. If it is assumed that the defect component is dominated by trapping to Cd vacancy defects and that the defect specific trapping

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coefficient is approximately $10^{15}\,s^{-1}$,[15] and a concentration of $\sim 4 \times 10^{16}\,cm^{-3}$ is obtained.

The temperature dependence of the mean positron lifetime, τ_m, is shown in Fig. 1. Positron trapping to negatively charged vacancy defects is expected to increase with reducing temperature proportional to $T^{-1/2}$,[8] so the mean lifetime is expected to increase toward the value characteristic of the vacancy defect with reducing temperature. There is evidence that the stable charge states of the Cd vacancy are negative.[1,3] The reduction in τ_m with reducing temperature observed in Fig. 1 has also been observed for Cl-doped and In-doped CdTe.[15,16] This temperature dependence provides clear evidence for trapping to defects with a small binding energy for positrons, and the associated positron states exhibit a lifetime similar to the bulk, perfect lattice, lifetime value, τ_B.[9,15] The fit to the STM for one vacancy defect ($\tau_v = 330$ ps) with one shallow binding energy trap ($\tau_{st} = \tau_B = 285$ ps),[15] both negatively charged, is shown in Fig. 1. Substitutional acceptor impurities have a negative charge and can localize positrons at low temperatures, but there is no associated open volume so their annihilation characteristics are similar to perfect lattice positron states. Other experimental methods commonly observe a shallow acceptor in CdTe which has been attributed to oxygen,[17,18] including the substitutional center O_{Te}.[19]

The vacancy defect lifetime and the calculated bulk lifetime, τ_B, values obtained here are in agreement with earlier studies of CdTe and $Cd_{1-x}Zn_xTe$.[15,16,20–29] Previous work has provided clear experimental evidence that τ_B lifetime of CdTe is in the range of 280–290 ps.[15,16,20,23–27] These studies also report a vacancy-related defect lifetime in the range ~315–395 ps, which unambiguously demonstrate that these samples contain open volume point defects.[15,16,20–27,29] Positron annihilation lifetime spectroscopy is of particular importance because of the ability to resolve several different positron states; however, if two lifetime components are to be resolved, the second must be sufficiently greater than the first or a single weighted average component will be obtained. This ability depends on spectrometer IRF, the number of counts, and the number of lifetime components in the spectrum and typically requires the second lifetime to be in the range ×1.3–1.5 greater than the first. Krause-Rehberg and coworkers[15,21] demonstrated that a defect lifetime in CdTe initial reported to vary in the range of ~350–395 ps was, when higher statistics spectra were analyzed, due to two components, one at 330(10) ps and a second at 450(15) ps. More recently, lifetime studies performed on CdTe thin films, free of source correction terms in the deconvolution, were best fitted with two defect lifetimes at 321(3) ps and 450(30) ps.[27] Both studies propose that the Cd monovacancy lifetime in CdTe is in the region 320–330 ps and that the ~450 ps lifetime component is due to divacancy defects.

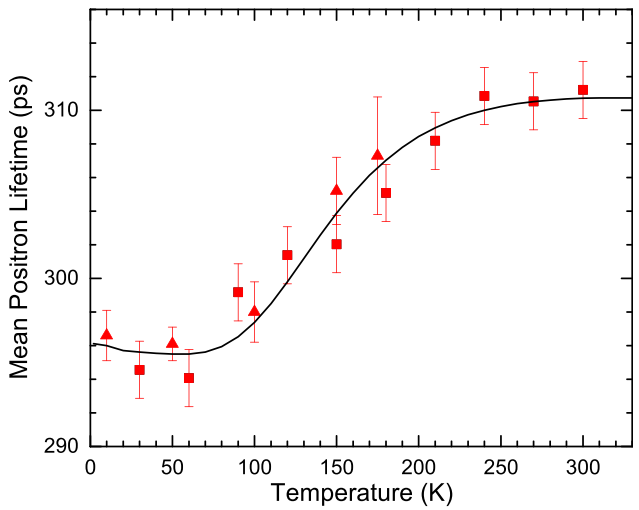

FIG. 1. Temperature dependence of the mean positron lifetime for Zn-doped, 0.15% by weight, CdTe single crystals. The standard trapping model fit line assumed a shallow binding energy trap ($E_b = 38$ meV) and a vacancy defect, both negatively charged.

The assignment of the ~320 ps defect lifetime to the Cd vacancy related defect was based on comparison with atomic superposition DFT calculated lifetimes.[27,30] Recent first-principles calculations of point defects in CdTe have provided further insight on local structure and stability.[1–5,31] Possible relaxed geometries of the two stable charge states, −1 and −2, of the Cd vacancy,[1,3] and for the −1 charge state of Cl-donor A-center, V_{Cd} with a Cl_{Te} nearest neighbor,[2] have been reported. The other point defect considered of particular importance in these materials is the Te antisite; this has also been studied and relaxed structures for the three charge states, Te_{Cd}^{+2}, Te_{Cd}^{0}, and Te_{Cd}^{-2}, given.[1,4] Importantly, it was found that both the neutral and −2 states of Te_{Cd} should be viewed as vacancy-interstitial complexes. Here, we perform atomic superposition DFT calculations of positron parameters to investigate both the possible influence of local relaxation on the annihilation characteristics of V_{Cd} and the possibility of positron trapping to the proposed vacancy-interstitial structures for Te_{Cd}^{0} and Te_{Cd}^{-2}. In addition, a recent DFT investigation of the Te vacancy has provided evidence for the possible importance of the +2 and neutral charge states.[31] Calculated positron parameters for V_{Te}^{0} are given.

The calculations were performed with the MIKA/Doppler package using 1000 atom supercells.[7,10,32] The electron-positron enhancement factor obtained from the data of Arponen and Pajanne,[33] both the original by parameterization by Boroński and Nieminen (BN),[34] described within the local density approximation (LDA), and with an expression obtained by Barbiellini and co-workers[35,36] (referred to as AP), described within the generalized gradient approximation (GGA) were used. The LDA calculations with BN enhancement assumed a value of 7.1 for the CdTe high frequency dielectric constant. The resulting positron lifetimes for the relaxed states of the relevant point defects are given in Table I, and the results for the perfect lattice, τ_B, and the unrelaxed monovacancy and divacancy defects are also included. The BN enhancement calculations underestimate the τ_B value, while the AP calculations over estimate it. Similarly, the BN enhancement values for the localized positron states are significantly lower than the observed experimental lifetime values.

The AP calculated value for the unrelaxed V_{Cd} is in good agreement with previously reported defect lifetimes.[15,27] For the −1 state of V_{Cd}, two possible electronic configurations were considered, the symmetric T_d symmetry state and the more stable polaronic C_{3v} state.[3] The C_{3v} state can be considered by assuming the polaron is localized on the "top" Te ion,

TABLE I. Positron lifetime values (ps) calculated by atomic superposition DFT for monovacancy, antisite, and divacancy defects in CdTe.

	Enhancement	Lifetime	τ_D/τ_B
Bulk	AP	309	
	BN	276	
V_{Cd}	AP	322	1.043
	BN	291	1.054
V_{Cd}^{-1} (T_d)	AP	312	1.010
V_{Cd}^{-1} (C_{3v})	AP	312	1.010
	BN	278	1.010
V_{Cd}^{-2} (T_d)	AP	311	1.007
$(Cl_{Te} - V_{Cd})^{-1}$	AP	323	1.046
Te_{Cd}^{-2}	AP	310	1.005
	BN	277	1.005
Te_{Cd}^{0}	AP	311	1.008
V_{Te}	AP	343	1.111
	BN	307	1.114
V_{Te}^{0} (C_{2v})	AP	348	1.125
$V_{Cd}V_{Te}$	AP	417	1.351
	BN	355	1.290

Te-1 in Fig. 2(a), the separation between the vacant Cd site and Te-1 decreases by 2.9% and the separation between the from the Cd vacancy site to the lower three Te ions reduces by 9.2%.[3] For the T_d symmetry -1 state, all four Te nearest neighbors move closer to the vacancy by 7.9%. The stable -2 state of V_{Cd} is also reported to retain T_d symmetry, and the Te ions relax by 9.4% toward the vacancy site.[1] The inward relaxations exhibited by the geometries of the -1 and -2 states of the Cd vacancy result in a similar reduction of the positron lifetime values by approximately 10 ps compared to the unrelaxed V_{Cd} (Table I).

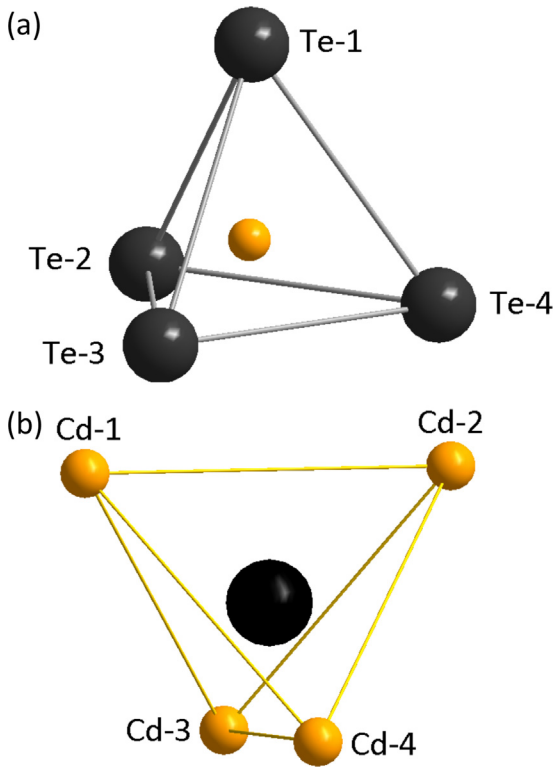

FIG. 2. Schematics of (a) the Cd site and (b) the Te site for the ideal CdTe lattice.

Given the importance of donor dopants, such as Cl and In, in modifying the properties of CdTe materials, the available structure for the -1 charge state of the Cl-donor A-center was also investigated.[2] The Cl_{Te} nearest neighbor is displaced away from the vacancy Cd site by 5.0%, while the three Te ions relax toward the site by 1.3% and the slight increase in the lifetime obtained (Table I), compared to the unrelaxed V_{Cd}, is consistent with these relaxations. The recently calculated structure for the neutral charge state of the Te vacancy (Fig. 2(b)) involved two of the neighbor Cd atoms relaxing away from each other, while the remaining pair form a dimer.[31] This configuration for V_{Te}^{0} gives a slightly increased positron lifetime compared to the unrelaxed V_{Te} (Table I).

It has been reported that the local structure of both the neutral and -2 charge states of the Te antisite have open volume.[1,4] For the neutral charge state, the Te at the original Cd site is displaced away from Te-1 (Fig. 2(a)) almost into the plane of lower Te atoms.[4] A split interstitial configuration is predicted for the -2 charge state, the antisite Te atom displaces on to the Te-1 to Te-2 line, and the Te-2 atom is displaced away from Te-1 along the same line.[1] The positron wavefunction exhibited localization, and the resulting positron lifetimes for the two charge states were found to be similar (Table I); these were again approximately 10 ps smaller than the lifetime for the unrelaxed V_{Cd} defect.

It should also be noted that if the relaxations toward the vacancy-interstitial geometry are smaller than predicted,[1] it is probable that the neutral and negative states of the Te-antisite would weakly bind positions and hence also be a candidate centers for shallow positron trap observed here.

Given the similarity between the obtained positron lifetimes for V_{Cd}^{-1}, V_{Cd}^{-2}, Te_{Cd}^{0}, and Te_{Cd}^{-2} (Table I), it is of interest to also calculate coincidence Doppler broadening ratio spectra; these are shown in Fig. 3. The spectra are the ratio of the momentum distribution obtained for the localized positron against the perfect lattice state distribution; both are convolved with a Gaussian representing a detector resolution of 1.1 keV.

Figure 3 shows the isolated V_{Cd} defect CDBS spectra have a characteristic peak at 20 mrad, and the ratio value of this peak is observed to increase for the relaxed geometries. The Te_{Cd} antisite spectra are different: they exhibit a less pronounced peak shifted to lower momentum value (Fig. 3(b)). It should be noted that the spectrum for the divacancy defect is characteristic, and it has a markedly lower ratio value and evidence of a peak shifted to high momentum compared to V_{Cd} (Fig. 3(a)).

The relaxed Cl A-center spectrum is also characteristically different from the V_{Cd} spectra, and there is a clear peak at 26 mrad, and the associated lifetime value is slightly larger than that for the unrelaxed V_{Cd}. The Te vacancy gives a larger lifetime than the V_{Cd} related defects (Table I), and again, the CDBS ratio spectra exhibit characteristic features; a minimum at approximately 20 mrad, the position of the peak in the V_{Cd} spectra, and a peak at approximately 28 mrad. The relaxation of V_{Te}^{0} [31] results in a slight increase in the lifetime and a similar CDBS spectrum but shifted to lower ratio value (Fig. 3(a)).

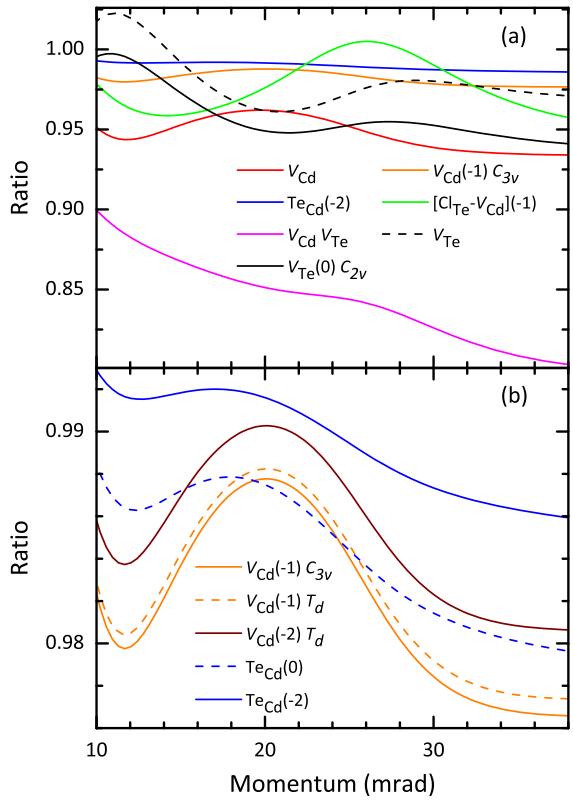

FIG. 3. Atomic superposition DFT calculated coincidence Doppler spectroscopy ratio spectra for various states of the monovacancy and Te antisite defects obtained using the AP enhancement factor. The Cl-donor A-center and the unrelaxed divacancy defect are also included.

Early CDBS measurements extending to 20 mrad were performed on Cl-doped and In-doped CdTe;[22] a minimum at approximately 13 mrad was observed for the Cl-doped samples, in good agreement with the calculated Cl A-center spectrum shown in Fig. 3(a). Normally, CDBS measurements provide spectra that extend beyond 30 mrad.[7]

The positron lifetime measurements can, importantly, resolve several positron states. For CdTe materials, there is good agreement on the experimental value for τ_B of ~285 ps, and a defect lifetime in region 320–330 ps is commonly observed. The defect lifetime is in agreement with the unrelaxed V_{Cd} value calculated with the AP enhancement (Table I), but the inward relaxations of Te nearest neighbors for the −1 state reduces the calculated lifetime by approximately 10 ps. It should be noted, however, that if the localization of the positron at the vacancy site is included self-consistently in the DFT approach, the presence of the positron may mitigate this inward relaxation.[37] The assignment of the 320–330 ps defect lifetime to V_{Cd} remains plausible, in particular, when, for example, in this study, the processing conditions are Te rich.[16,21] Further, the calculations presented here admit the possibility of positron trapping to the vacancy-interstitial geometries of Te^0_{Cd} and Te^{-2}_{Cd}.[1,4] These configurations of the Te antisite give the similar lifetime values the relaxed configurations of V^{-1}_{Cd} and V^{-2}_{Cd}, and so introduce a possible ambiguity in the assignment of the defect with a lifetime of ~320 ps. However, the differences observed between the calculated CDBS ratio spectra, shown in Fig. 3, demonstrate the potential of combined CDBS and PALS measurements to differentiate between V_{Cd} and Te_{Cd} type defects, as well as identify other technologically important point defects in CdTe materials.

In summary, this work demonstrates that the positron lifetime spectra from lightly Zn-doped CdTe, prepared with using a small Te excess, exhibit similarities to studies of other doped and undoped CdTe samples;[15] a vacancy defect with a lifetime of ~330 ps is observed, and the temperature dependence of the mean lifetime (Fig. 1) shows that trapping to weak binding energy defects, with positron states similar to the bulk, onsets at low temperatures. The observation of vacancy defect positron trapping is unambiguous. The capability of PALS to resolve different positron states, rather than provide an average due to all states present, is of particular importance. But, as noted above, there are limits on this ability. The DFT calculated positron lifetime values using relaxed geometries of the relevant point defects in CdTe presented here demonstrate that positron trapping may occur both at vacancy defects, but also at proposed vacancy-interstitial configurations of Te_{Cd} antisite defects,[1] and show that several different point defect states, e.g., V^{-1}_{Cd}, V^{-2}_{Cd}, Te^0_{Cd}, and Te^{-2}_{Cd}, may exhibit comparable lifetime values (Table I). These results motivated an extension of the DFT study to the calculation of coincidence Doppler broadening ratio spectra for the same point defect configurations (Fig. 3). Clear differences in the CDBS ratio spectra were obtained for the different vacancy defects and for Te_{Cd} antisite trapping. We present evidence that combined PALS and CDBS experiments have the capability to detect, identify, and quantify primary technologically relevant point defects in CdTe. Processing protocols are commonly designed, in part, to suppress inferred relevant point defects, progress in unambiguous experimental identification in device, or near device, material is of clear importance. Facilities are in place that enable both PALS and CDBS to be performed on thin films,[38,39] in addition to the more widely available conventional studies of bulk samples.

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